



no.2²⁰¹⁷

PDC Center for High Performance Computing

PDC Newsletter

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Erwin Laure
Director, PDC

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PDC operates leading-edge, high performance computers as easily-accessible national resources. These resources are primarily available for Swedish academic research and education. PDC, which is hosted by CSC, KTH, is one of the six centres in the Swedish National Infrastructure for Computing (SNIC).

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Cover

Thanks to Scania, Beskow was upgraded at the end of August with an extra two cabinets, thus increasing the theoretical peak performance from 1.97 to 2.44 PFLOPS. Here Cray staff are bringing one of the new cabinets into the PDC computer hall via the lift.

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Editorial

Collaboration with industry is an important aspect of PDC to facilitate technology transfer from academia to industry and foster the uptake of high-performance computing (HPC) in industrial settings. A highlight of these collaborations is our engagement with Scania, which has developed into a very close collaboration over several years. This summer Scania invested heavily in our flagship system, Beskow, and, thanks to this investment, Beskow has been upgraded to a total capacity of 2.5 petaflops. You can read more about Scania's HPC usage and the Beskow upgrade in our cover story. Also mark your calendars for the upcoming PDC Industry Day on the 1st of March 2018.

The main focus of PDC is clearly to support academic HPC users. Although we do provide Swedish researchers with excellent hardware resources, some have even greater needs that cannot be met nationally. This is why we are a member of PRACE: to provide Swedish scientists with the possibility to access the largest European HPC systems. Four large-scale Swedish PRACE applications have been granted lately, as well as a number of smaller DECI and industrial allocations.

During the autumn we have continued our education programme, with the PDC summer school being a particular highlight, and the CodeRefinery project has had their first set of workshops. Together with the Swedish e-Science Research Centre (SeRC) we have started a new initiative – the PDC-SeRC seminar series; these seminars highlight innovative research using HPC. The BioExcel project has recently organized their first Community Forum, and we are also hosting our first visitors at PDC through the HPCE3 programme.

When PDC retires computer systems, their components are typically recycled. But sometimes these systems also see a new life at another place. This summer we were able to donate parts of our old "Ekman" system to the University of Sarajevo, supporting their efforts in educating the next generation of computational researchers.

Finally, the implementation of SNIC 2.0, the next phase of the Swedish National Infrastructure for Computing (SNIC), is making good progress. With the approval of the next round of funding by the Swedish Research Council (VR), a major milestone has been met and now the SNIC universities are finalizing their collaboration within SNIC 2.0. This means that for the next couple of years the continued operation of SNIC is guaranteed and Swedish researchers will continue to have access to leading HPC systems for their work. With this good news, I would like to wish all PDC users "God Jul & Gott Nytt År"!

Erwin Laure, Director PDC



PDC-Scania Collaboration

Mattias Chevalier, Scania

Scania has been in a strategic partnership with PDC since 2010 and thanks to this collaboration, Scania has access to world-class high-performance computing (HPC) resources. As a manufacturer of heavy commercial vehicles, Scania naturally has large in-house computational resources to carry out various forms of simulation studies covering many different disciplines, for example, finite element method (FEM) and computational fluid dynamics (CFD) simulations. Running benchmarking performance tests on a larger system than we could motivate to host on our own gives important input when extending in-house computer cluster resources. A massively parallel system is of great use when it comes to balancing peak load situations, and also when fast turnaround times are needed.

The large number of cores accessible through the collaboration with PDC has become an important and necessary asset in order for Scania's R&D organization to deliver simulation results in time. To date several software applications have been used, but our primary focus has been on computational fluid dynamics (CFD) simulations using the tools PowerFLOW, OpenFOAM and STAR-CCM+. Many simulations have been dedicated to studies of complete vehicles



Above: Volume rendering of the instantaneous velocity magnitude on the leeward side of an R20 Highline truck at crosswind conditions (Source: Scania)

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where different vehicle properties have been optimized. Performance evaluations of more tools are currently ongoing and the range of software we utilize will most likely be increased in the near future. Our collaboration with PDC also simplifies the dialogue process with other experts in the area and thus promotes effective and efficient knowledge transfer.

Simulation has become an important component of the product development process at Scania. By validating early designs through simulations, costly problems later in the development process can be avoided. In addition, simulations can be used to evaluate a larger range of concepts in order to optimize the most important properties of the products. Utilizing high-performance computing resources for simulation-based product development has enabled Scania to shorten lead times in our development process while building fewer physical prototypes and also improving both the quality and properties of our products.

In light of the benefits of the collaboration to date, Scania and PDC have agreed to continue our cooperation in the area of high-performance computing, focusing on the following areas:

- implementing related research and development projects with a focus on solving technical problems, developing methods and so forth,
- exchanging relevant HPC skills and knowledge,
- undertaking thesis work and support of postgraduate education in the HPC area, and
- making computing capacity at PDC available to Scania. The collaboration currently co-funds part of Beskow, PDC's Cray XC40 cluster, which corresponds to approximately 16,000 cores of continuous running.

“The collaboration with PDC has significantly decreased the turnaround time for large-scale simulations both due to the large capacity of the systems at PDC and due to assistance from PDC's HPC experts,” says Magnus Pettersson, Engineering Director at Truck Chassis Development at Scania.

Upgrade of Beskow

Gert Svensson, PDC

Due to the **continued and increased collaboration with Scania**, the PDC main system, Beskow (which is a Cray XC-40), has been upgraded with the addition of two further cabinets. The nodes that make up the new cabinets are all equipped with a new version of Intel processor and also have more memory than the CPUs in the original Beskow nodes.

Following the upgrade, Beskow consists of eleven cabinets with a total of 515 blades; this gives an overall total of 2,060 compute nodes, each with dual Intel CPUs. The nine old cabinets have Xeon E5-2698v3 Haswell 2.3 GHz CPUs (16 cores per CPU) and the two new cabinets have Xeon E5-2695v4 Broadwell 2.1 GHz CPUs (18 cores per CPU). This means that Beskow now has 67,456 cores in total.

Overall Beskow's theoretical peak performance has increased from 1.97 to 2.44 PFLOPS, and its performance in the LINPACK benchmarks has gone from 1.40 to 1.80 PFLOPS. During the LINPACK run, the system consumed an average of 842 kW of power compared to around 720 kW in normal operation.

At the time of writing, the scheduling of jobs on the new system is still undergoing testing. Normal computing jobs can be scheduled on the new nodes, although Scania jobs have priority on the new nodes (and may also be scheduled on the old nodes).

The extended research collaboration with Scania was discussed during the spring of 2017 and an official agreement was formalised on the 26th of June 2017. PDC had already discussed the contract for an extension of Beskow with Cray, so we were able to order the upgrade to the system on the 29th of June. The system was promptly installed starting on the 30th of August. As is usual with Cray systems, this was a well-planned, highly efficient operation. The upgrade was accepted on the 13th of September and user jobs immediately started being run on the upgraded system.

Beskow Being Upgraded



Above: Each compute rack arrives packed in a crate. Here one of the crates is lifted from the delivery truck with a forklift.



Above: The racks (in their protective crates) barely fit through the doorway to the entrance area of the PDC computer hall.



Above: The crates are removed before the racks are taken into the computer hall. See cover image for getting up the stairs!



Above: Each rack is moved into the computer hall using metal sheets to protect the floor and distribute the weight.



Above: It requires several people to move the racks to their final positions.



Above: Finally Cray staff and PDC staff work together to connect the new racks as part of the Beskow system.

PDC Tightens Collaboration with Swedish SMEs


Lilit Axner, PDC

In 2017 PDC continued to deepen its relationship with industrial high performance computing (HPC) research and development (R&D). Several more Swedish small to medium-sized enterprises (SMEs) started new collaborations with PDC, while our relationships with already established SME partners have been expanded. Moreover, several more SMEs have successfully explored the HPC possibilities that are offered by such EU projects as PRACE and HPC-Europa3.

However, it has been some time since PDC intensified its collaborations with Swedish SMEs (and industry in general), and thus it is now time for us to continue this activity in a more coordinated and informative manner. Consequently we will be hosting a special event early next year that is designed specifically for large industrial concerns, independent software vendors (ISVs) and SMEs – the event will be known as the “PDC Industry Day” and we hope to continue hosting this event on an annual basis. Note the details below so you can save the date in your diary.

PDC CENTER FOR HIGH PERFORMANCE COMPUTING

**SAVE THE DATE:
PDC INDUSTRY DAY**




DATE: 2018-03-01
TIME: 10:00 AM
**PLACE: OPENLAB
MULTIPURPOSE HALL**

**ADDRESS:
VALHALLAVÄGEN 79,
114 27 STOCKHOLM**

HAVE YOU EVER THOUGHT OF COMPETING ON THE INTERNATIONAL MARKET? - THEN HIGH PERFORMANCE COMPUTING IS YOUR KEY TO IT.

COME AND LEARN ABOUT SUCCESSFUL EXAMPLES OF INDUSTRIAL USE OF HPC AND GET ACQUAINTED WITH THE LARGE RANGE OF EASY-TO-USE HPC SERVICES PROVIDED BY PDC TO INDUSTRY.



SCANIA – PDC'S LARGEST INDUSTRIAL PARTNER
VOLUME RENDERING OF THE INSTANTANEOUS VELOCITY MAGNITUDE ON THE LEEWARD SIDE OF AN R20 HIGHLINE TRUCK AT CROSSWIND CONDITIONS

Right: The PDC Summer School "Introduction to High Performance Computing" is held each year in Stockholm at the end of the summer. As part of the school, the students are given a tour of the PDC computer hall in small groups of up to ten people. Gert Svensson, the Deputy Director of PDC, shows each group the computing systems and storage, as well as pointing out parts of the supporting infrastructure, such as the backup power supply. Here is one of the groups from the 2018 Summer School in front of Beskow, PDC's flagship system (which was just about to be upgraded).
PDC computer hall, 15 August 2017

Introduction to PDC Systems Course

Thor Wikfeldt, PDC

The course “Introduction to PDC Systems” is held twice each year (usually at the start of the year in February and then after the summer break, either in September or October) and serves to introduce researchers to the fundamentals of high performance computing (HPC), while focusing particularly on the HPC infrastructure at PDC. The topics that are covered in the course include:

- background information about HPC and PDC,
- information about the computer clusters available at PDC,
- how to apply to use PDC resources,
- how to get a PDC account and log in to PDC clusters,
- how to run software on different nodes at PDC,
- how to efficiently store your research data, and
- how to compile code at PDC.

The second introductory course for 2017 was held at PDC on the 5th of October and was attended by ten researchers. Slides from the course are available [here](#). In addition to going through the prepared material, course participants were able to get assistance to set up their laptops for logging in to PDC, and there was also a live demonstration (where participants could type along on their own laptops) of common procedures and commands that are used when working on the PDC systems.

The next introductory course will be held in February 2018. So, if using the PDC systems is new to you, it is highly recommended that you attend the course since it is likely to significantly speed up the process of becoming comfortable with working in the HPC environment at PDC! To find out the date for the course, either [join the PDC announcements mailing list](#) or watch the [PDC Events calendar](#) or follow [PDC on Facebook](#).



Staff Focus



Mao-Wei Nilsson

Mao-Wei is a fifth-year student who is currently in the Systems, Control and Robotics programme at KTH. She studies courses such as control theory, machine learning, and deep learning. While she has been studying, Mao-Wei has worked part-time as a lab assistant for programming in Python and C, and as a web designer. Before she started studying Electrical Engineering, Mao-Wei already had a Masters degree in econometrics, and had worked as a research fellow within the econometric field.

At present Mao-Wei is working at PDC in first-line support. She also works with documentation about PDC resources on the PDC website.

Mao-Wei's hobbies include watching movies, cooking, and spending time with her cats and family.



Above: PDC Summer School Picnic, 14 August 2017

Staff Focus



Charles Kinuthia

Charles Kinuthia started work at PDC Support early in 2017. Charles is doing a five-year programme at KTH and is currently in his last year of an M.Sc. in Systems, Control and Robotics. Charles moved from Kenya to Sweden 10 years ago. He will soon start a Masters thesis project in deep learning.

Charles has a passion for programming; he enjoys working on his own programming projects and has previously worked as a teaching assistant in a programming course. This passion is why he loves working at PDC where he has had the chance to learn more about parallel computing. Other activities that Charles enjoys include playing video games and going to the gym.



Above: 3rd PDC-SeRC Seminar, PDC, 24 November 2017

HPCE3 Visitors at PDC

Lilit Axner, PDC

In the [previous edition of this newsletter](#), we announced that a new four-year-long transnational access project called **HPC-Europa3** (or **HPCE3**) started on the 1st of May 2017 and that PDC is one of the ten main partners representing Sweden in this project. The project is based on a programme of visits, in the form of traditional transnational access, with researchers visiting high-performance computing (HPC) centres and/or scientific hosts. The visitors are funded for **travel, accommodation and subsistence**, and provided with **an amount of computing time** suitable for their approved project.

In this project PDC has committed to host about 40 visitors from all over the world, although prioritization will be given to visitors from the Baltic countries. The aim is to tighten the collaboration between the Baltic countries and Sweden, as well as to promote the use of HPC in the Baltic countries.

HPCE3 calls for applications are always open, however there are four cut-offs per year. Currently HPCE3 is accepting applications for the third cut-off that will end on the **28th of February 2018**.

For the first call, HPCE3 received 70 applications, 52 of which were accepted. In the second call, HPCE3 received 22 applications and the results of the second call will be known in December. PDC received 4 applicants per call in both of these calls. The applicants were from Lithuania, Latvia, Greece, Slovenia, Belarus, Switzerland, Serbia and Denmark.

Currently we are hosting our first visitor, Dr. Shannon Stauffer from the Center for Physical Sciences and Technology in Lithuania, who is collaborating with Prof. Natalia Skorodumova from the Department of Materials Science and Engineering at KTH. The duration of the visit is five weeks during which time they will be investigating the mixed metal NASICON for Na-ion battery electrodes by running Vienna Ab initio Simulation Package (VASP) simulations on Beskow at PDC.

The other three visitors who were accepted in the first call will be arriving at PDC in January 2018.

If you are involved in a collaborative project with researchers from any other country (especially with one of the Baltic countries) then HPCE3 is a unique opportunity for you to invite your collaborative partners to visit Sweden and enhance their research by using the supercomputer Beskow at PDC. HPCE3 will cover their travel and accommodation costs and also provide a modest subsistence allowance.



PDC-SeRC Seminar Series

Thor Wikfeldt, PDC

Since earlier this autumn, PDC and the Swedish e-Science Research Centre (SeRC) have been hosting a new series of seminars about e-Science where SeRC members and other interested researchers and students can meet to exchange ideas and listen to inspiring e-Science presentations by outstanding researchers. The seminars take place each month in the SeRC Open Space on the fifth floor of Teknikringen 14 (which, for those who have not visited us yet, is the home of PDC). This space, which was inaugurated last year, is designed to promote interactions between researchers from various scientific domains, computer scientists, and high performance computing (HPC) practitioners - an objective which has been nicely actualized by the new PDC-SeRC seminar series.

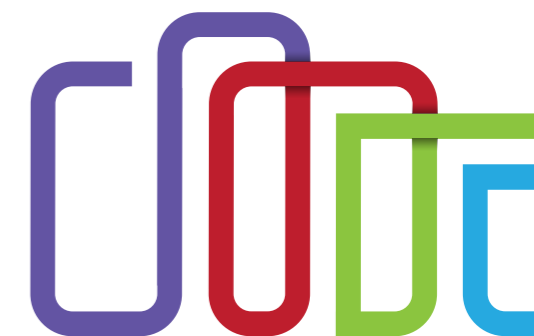
All seminars take place during lunchtime (that is, from 12:00-13:00) and participants can enjoy a light lunch along with coffee and tea - this format creates an informal atmosphere which stimulates free interactions with plenty of questions and discussions. The first three seminars in this series have been:

1. "Building machines that understand human body language" by Prof. Hedvig Kjellström from the Robotics, Perception and Learning (RPL) lab at KTH, 28 September,
2. "Feature-based Visualization" by Prof. Tino Weinkauff from the Visualization and Data Analysis laboratory, KTH, 23 October, and
3. "An insight into computational proteomics" by Prof. Lukas Käll from the Science for Life Laboratory, 24 November.

The new seminar series has been well received by people in the e-Science research communities,

and PDC, together with SeRC, plans to continue with these monthly seminars in 2018, inviting outstanding researchers from various disciplines to present exciting results from the forefront of their research fields. We hope that this initiative will grow into an established tradition in Swedish e-Science and contribute to inter-disciplinary collaborations and cross-fertilization of ideas.

We welcome you to attend the seminars when they start again in January 2018. All the seminars will be advertised on the PDC website, but if you would like to receive email announcements, please contact Thor Wikfeldt (kthw@kth.se), PDC's local organizer. Finally, we also welcome volunteer speakers, so please get in touch if you are interested in giving a PDC-SeRC seminar!



CODE REFINERY

First Year of CodeRefinery

Thor Wikfeldt, PDC

Is there room for improvement in how scientific code is developed in academia? Nowadays developing software forms a cornerstone of research projects conducted across a wide range of scientific disciplines, but researchers often lack training in modern methods and tools for software development. The **CodeRefinery project**, which was launched last autumn under the umbrella of the Nordic e-Infrastructure Collaboration (NeIC), is founded on the principle that better software leads to better research, and that it is never too late for a researcher, nor is it ever too early, to adopt better practices in day-to-day code development. A core aspect of the project is to organize and teach concise three-day workshops on collaborative, sustainable scientific software development.

The aim of these workshops is not only to bring researchers up to date with modern tools and practices, but also to encourage researchers to share with colleagues what they have learnt when returning to their home institutions and thus, in the long run, to contribute to an improved culture in research software development. In addition to delivering workshops, CodeRefinery has set up a free platform for distributed version control of public and private code. This repository hosting service, based on a GitLab instance, is open to researchers based in the Nordic countries and is available at <https://source.coderefinery.org>.

Now, in its second year, CodeRefinery leaves behind an eventful first year packed with workshops, course material development, infrastructure building for source code hosting and community engagement. Workshops have so far been held in Helsinki, Stockholm, Copenhagen, Tromsø, Aarhus and Linköping, and in addition shorter workshops and discussion meetings have been held in Oslo, Umeå and Stockholm, along with a sister event in Manchester, UK. The majority of workshop attendees have been Ph.D. students and postdoctoral researchers who need to write code or scripts for research, but many participants have been either more junior or more senior. A key question for the project, as it now enters its second year, is whether the workshops have been successful in bringing about a positive change in how research code is developed. To shed light on this question a post-workshop survey was conducted, and the results have been encouraging: over 80% of former participants report that their code is both more reusable and more reproducible, 78% report that it has become easier to collaborate on software development with colleagues, and 62% report that they have introduced one or more colleagues to new tools or practices. The graph below shows how survey respondents evaluate the impact of attending a CodeRefinery workshop on their usage of various software development tools. Version control with Git is a core topic in CodeRefinery workshops, and the graph below shows that this makes a large impact on the work of workshop participants: 65% report that their

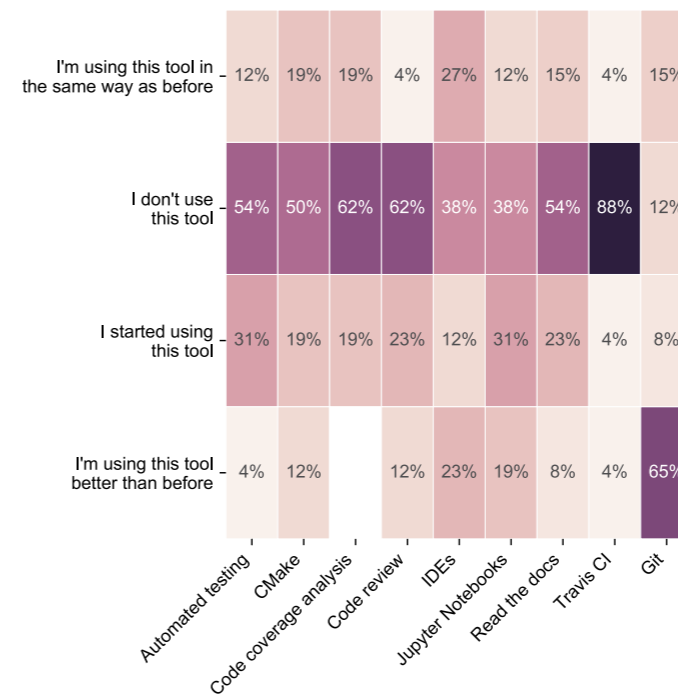
usage of Git improved after the workshop. Even other topics, which due to time constraints take up less than 2 hours of the 3-day workshop schedule, have had a significant impact. Automated testing and Jupyter Notebooks have been adopted by 31% of former participants, and 23% report that they have started using code review and the Read the Docs platform in their projects.

The second year of the CodeRefinery project will also be its last, at least in its current form, but a follow-up project is in the pipeline. However, a major challenge for a CodeRefinery-2.0 project will be how to scale up. Funding will remain restricted to providing a handful of instructors and, based on our experience up to now, this has not been enough to meet the demand. An interesting future prospect is for the CodeRefinery workshops to grow into a community initiative based on voluntary efforts by motivated individuals in the academic world who want to make a positive impact on the quality of research software. That this is not an unattainable goal is demonstrated by the success of the [Software Carpentry project](#), which has been teaching basic computing skills to researchers since 1998, and whose instructors are, without exception, “regular” academics who enjoy teaching and find it meaningful to share their expertise with fellow researchers (and in doing so pick up new skills themselves!).

Before these issues become urgent questions, CodeRefinery members have much to look forward to. Workshops are being planned for Helsinki in December 2017, and in 2018 the project will visit Trondheim, Turku, Odense, Uppsala, Oslo and, finally, Reykjavik in the late summer. If you want to attend a workshop, visit the project website (where you can sign up to be notified of future workshops in your area - see coderefinery.org/workshops). If you are interested in helping out and/or getting involved in the project, get in touch via the support line, support@coderefinery.org, or via the mailing list, <https://groups.google.com/group/coderefinery>.

Until then, good luck with your software projects from all of us at CodeRefinery!

Below: Post-workshop survey results showing how attending a CodeRefinery workshop has influenced the usage of various software development tools



Swedish PRACE Successes

Lilil Axner, PDC

The second half of 2016 and the year 2017 have been very successful for Swedish researchers in the PRACE research infrastructure projects. Specifically we have shown excellent results in the following activities.

There have been four successful Tier-0 projects for the PRACE project 14th and 15th calls, two per call. The projects are as follows.

- 1. HETS/Heat (and Mass) Transfer in Turbulent Suspensions**
Project Leader: Prof. Luca Brandt, KTH
Resource Awarded: 18.3 million core hours on Marconi – KNL
- 2. Direct numerical simulation of partially premixed combustion in internal combustion engine relevant conditions**
Project Leader: Prof. Xue-Song Bai, Lund University
Resource Awarded: 42.4 million core hours on Juqueen
- 3. BioTitan – Ab initio molecular dynamics of biomolecular adsorption on fully hydrated TiO₂-water interfaces**
Project Leader: Prof. Alexander Lyubartsev, Stockholm University
Resource Awarded: 50.2 million core hours on MareNostrum
- 4. Large-Eddy-Simulations of the unsteady aerodynamics of oscillating airfoils at moderately high Reynolds numbers**
Project Leader: Prof. Dan Henningson, KTH
Resource Awarded: 40 million core hours on Hazel Hen

Website Update

Gert Svensson, PDC

The PDC web site has been totally re-implemented over the summer and autumn. In the process, all the pages have been reviewed and updated. In particular, many of the support pages have been rewritten from scratch.

The website is now mainly based on the Polopoly framework that is used by the rest of KTH. This has several advantages - it means our pages now have a modern design with the same look and feel as the rest of the KTH web pages. A plus is that we can now easily share content and events with other KTH sections and departments.

As a matter of interest, the support section (that is, the technical documentation) is maintained in the Sphinx framework and imported into the KTH Polopoly system. (You may notice that the formatting of the Support pages is slightly different from the other pages on the updated website.)

Working with a website is an ongoing process, so if you have any comments or suggestions for improvements to the updated pages, please send them to webmaster@pdc.kth.se.



Above: Home page of the newly updated PDC website

Staff Focus



Szilárd Pall

Szilárd Pall studied computer science and received a Bachelor's degree in computer science at the Babeş-Bolyai University in Romania, and later a Master's degree in the same field from the Johannes Kepler University in Austria.

During the latter, and the following research engineering industrial position, he took his first steps into the world of scientific computing and gained early experience with GPU computing. To marry his passion for high performance computing with scientific challenges, he joined the graduate programme in computational biophysics in the group of Berk Hess and Erik Lindahl to work on parallel algorithms and methods for molecular dynamics.

Szilárd has helped redesign the parallel algorithms at the heart of the heterogeneous GPU acceleration in GROMACS and has been working as a member of the core developer team of this large FOSS community package.

Focussing on future-proof algorithms for wide SIMD and accelerator architectures his research brought great performance advantages, across

...continued on page 13

For the DECI 14th call there have been two successful Swedish projects as follows.

1. *CHARTERED2 - CHARge TransfER dynamics by time dependEnt Density functional theory*

Project leader: Dr. Biplab Sanyal, Uppsala University
Awarded hours: 29,904,000 DECI standard hours on Salomon, VSB-TUO, Czech Republic

2. *MMICSCTSET - Multiscale Modelling of Ionic Conductors – Structure, Conductivity and Thermodynamic Stability at Elevated Temperatures*

Project leader: Prof. Natalia Skorodumova, KTH
Awarded hours: 23,284,800 DECI standard hours on Salomon, VSB-TUO, Czech republic

As a consequence of these awards, seven projects from the Netherlands, the UK and Finland have been granted the use of an equivalent number of DECI standard hours on Beskow at PDC.

Sweden's successes in the industry-related activities within PRACE have also continued. For the PRACE SHAPE 5th call, the application by Svenska Flygtekniska Institutet has been approved for a project called "AdaptiveRotor". One of the PRACE application experts at PDC, Dr. Jing Gong, will be working in tight collaboration with the project investigator, Dr. Tomas Melin, for three months on performance and optimisation questions.

Two more applications from Swedish small to medium-sized enterprises (SMEs) have been accepted for the PRACE Type-D call. One of them is from Adaptive Simulations and the other is from Airinnova. These two SMEs have been awarded computing hours on the system called Archer at EPCC, UK.

There have also been several successful applications by projects with Swedish principal investigators to the PRACE preparatory Access calls.

This year PDC continued to be active within the PRACE dissemination and training activities. One of the major events was the hosting of the PRACE Spring School in the life sciences, "HPC for Life Sciences", in April 2017, which was undertaken together with the BioExcel Centre of Excellence.

We hope that in 2018 Swedish researchers will continue to apply to use the PRACE resources and that they will be as successful next year as they were in 2017. During the first half of 2018 we also plan to host a couple of PRACE workshops and training events in collaboration with the other Swedish National Infrastructure for Computing (SNIC) centres involved in PRACE.

PDC Donates Supercomputer to University of Sarajevo

Dejan Vitlacil, PDC

PDC and the KTH Royal Institute of Technology have donated a supercomputer for teaching purposes to the Faculty of Electrical Engineering (also known as ETF) at the University of Sarajevo. The system has recently been delivered and installed at ETF. This project was undertaken by PDC and KTH in conjunction with the **APU network** (a non-profit-making organization that contributes to positive development in Bosnia-Herzegovina and Sweden within the spheres of education, entrepreneurship, culture and sports). As you can imagine, moving a supercomputer to another country is a complicated task, so everyone in the project was grateful to the Embassy of Bosnia and Herzegovina in Sweden for providing administrative assistance with the undertaking, and to the Swedish company **Plivit Trade** who very kindly donated transport and other services vital for the relocation.

The supercomputer system that was donated to ETF consists of twenty multiprocessor server machines connected with an Infiniband network, along with suitable cabinets to accommodate and efficiently cool all the components. This is the first supercomputer with such a configuration to be hosted at a university in Bosnia and Herzegovina. Thanks to this donation, the University of Sarajevo has now joined the ranks of reputable university centres in the region that have a supercomputer infrastructure (such as Belgrade, Zagreb, Ljubljana and Sofia).

The supercomputer had previously been part of PDC's "Ekman" system, and the cabinets that the system is now housed in at ETF were part of the old computer room at the KTH School of Computer Science and Communication (CSC) before it was decommissioned. However, the real value of the supercomputer that has been given a new lease of life is more than just the market value of its components: the system will provide many students with a better education by giving them direct practical experience in the area of parallel computing. (Two young researchers from ETF have already attended the PDC Summer School "Introduction to High Performance Computing", so they will be ready to put the system to use straight away!) In addition to being used for teaching, the system will be utilised for research involving simulations, as well as data mining and other compute-intensive operations. Although the system is housed at the Faculty of Electrical Engineering, the supercomputer will be available to members of other faculties at the University of Sarajevo, which will maximise the benefits of the supercomputer system for both teaching and research at the university.

Staff Focus

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a wide range from workstations to large HPC machines, to the large research community of the GROMACS simulation software.

Since joining PDC in 2016 as a research engineer part of the SSF Research Infrastructure, he has been tackling the parallelization challenges of next-generation HPC architectures with a focus on molecular dynamics, in particular task scheduling on dense GPU accelerated machines. Szilárd is also an active member of the Swedish e-Science Research Centre Exascale Simulation Software Initiative (SESSI) group. In his free time, he is passionate about riding bicycles (even in the Swedish winter!).



Dan Lillrank

Dan Lillrank started at KTH first by enrolling in a B.Sc. in Engineering Physics, and is currently in his last year in the M.Sc. System, Control & Robotics programme at KTH. He works part-time in first-line support at PDC, and helps with the documentation of the PDC home page and general support duties. In his free time, Dan enjoys hanging around with friends, playing computer games and watching movies.

Below: Delivering the “recycled” supercomputer to the University of Sarajevo



PDC Summer School 2017

Stefano Markidis, CST

The latest PDC Summer School on “Introduction to High Performance Computing” took place from the 14th–25th of August 2017. The PDC Summer School provided students with a series of introductory lectures about computer architecture, parallel programming models (for shared and distributed memory systems, and for accelerators), and performance monitoring and analysis. The lectures were held in the mornings and were combined with hands-on exercises in the KTH computer labs during the afternoon sessions – during these the attendees ran parallel codes on both the Beskow and Tegner supercomputers at PDC. The lectures were given by experts in the parallel computing field, including Prof. Erwin Laure (KTH), Prof. Erik Hägersten (Uppsala University), Prof. Christoph Kessler (Linköping University) and Dr. Pekka Manninen (CSC-IT Center for Science, Finland).



Above: PDC Summer School 2017 group photo in the KTH courtyard

Below: Summer school lectures 2017



Fifty researchers and students, mainly from Sweden but also from other European countries (such as Spain and Denmark), participated in the PDC Summer School. The students were from both Masters and Ph.D. programmes in several fields, ranging from computer science to physics and electrical engineering to applied mathematics. This year’s PDC Summer School received excellent reviews from the attendees who highly recommended the course to their peers in the final evaluation. Among the many positive comments were ones such as: “The courses are all well organized and the labs at afternoon are really helpful. The lab assistants are all very patient.”, and “Excellent course. Will recommend to peers.”.

We are now preparing the PDC Summer School 2018 and any researchers (from academia or industry) who are interested in gaining a solid grounding in using high-performance computing for their research are warmly invited to attend. The school will be held in the last two weeks of August 2018, and further details will be available in Spring 2018.



Above: Guided tours of the PDC computer hall during the 2017 Summer School

Note: The photos of the 2017 PDC Summer School in this newsletter were taken by Sergio Rivas-Gómez from CST, KTH.

BioExcel Community Forum 2017

Rossen Apostolov, PDC

Conferences are great for learning what is happening in your field, meeting people in the coffee breaks (often your own colleagues!) and discussing the quality of the local catering services. We, at BioExcel (the European Centre of Excellence for Computational Biomolecular Research, which is led by PDC), decided to organize our community forum this year in a slightly different style.

First, the venue: the **Lloyd Hotel** in Amsterdam is not your regular hotel. Decades ago it used to be a place for refugees, later it was a prison, and eventually it was labelled a “Heritage” and turned into a hotel with a slightly “unusual” design. Let us leave the classification of the decor to the art experts but the bottom line is – with its creative interior – the hotel offered the perfect place for the kind of activities that we planned.

The forum brought together members of all the **BioExcel interest groups** and our own experts to discuss free energy methods, hybrid modelling, workflows, best practices for training and more, during several parallel sessions. The rather informal gatherings were of great value for everyone. New project ideas were discussed, and several of them were picked up for starting new collaborations. Our partners from Utrecht University brought along a great virtual reality (VR) kit that let you explore your favourite proteins in 3D while sipping a hot cup of coffee. The feedback from all the participants was incredibly positive so we had no choice – next year we will be doing it again! So you can start booking your cheap flight to Amsterdam now.

Meanwhile, to keep in touch with the upcoming BioExcel activities and our great team, visit www.bioexcel.eu and subscribe to our monthly newsletter. (We do not spam.)

PDC-Related Events

Cray User Group Meeting

20-24 May 2018, Hotel At Six, Stockholm

<https://cug.org/CUG2018>

PDC Industry Day

1 March 2018, Openlab (at KTH), Stockholm

For more information, join the [PDC Business mailing list](#) or watch the [PDC Events calendar](#) or follow [PDC on Facebook](#).

PDC Summer School 2018

Last two weeks in August 2018, KTH, Stockholm

In the spring of 2018, further information, including details about registration, will be available from <http://www.pdc.kth.se/training/pdc-summer-school>.

HPC Sources

We recommend the following sources for other interesting HPC opportunities and events.

CERN

<http://cerncourier.com/cws/events>

<https://home.cern/scientists/events/computing>

EGI

<https://www.egi.eu/category/events>

HPC University

<http://www.hpcuniversity.org/events/current/>

HPCwire

<http://www.hpcwire.com/events>

NeIC

<http://neic.nordforsk.org>

PRACE

<http://www.prace-ri.eu/HPC-access>

<http://www.training.prace-ri.eu>

<http://www.prace-ri.eu/events>

<http://www.prace-ri.eu/news>

SeSE

<http://sese.nu>

SNIC

<http://www.snic.se/news-events>

<http://docs.snic.se/wiki/Training>

XSEDE

<https://www.xsede.org>



Above: BioExcel Community Forum